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CALCULATION OF NEUTRON THERMALIZATION BY LAGUERRE POLYNOMIALS APPROXIMATION

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Abstract

An attempt is made to solve the thermalization problem in a homogeneous, infinite multiplying medium by using Laguerre polynomials approximation.

The whole energy range of neutrons is divided into two parts, namely the slowing down and the thermal region. The thermal flux is expanded into a series of Laguerre polynomials. The neutrons scattered from the slowing down region are considered as the thermal neutron source. The contact line between the two regions determines the so-called cut-off energy E_c. A comprehensive treatment for determining the source term and the cut-off energy is given. The thermal neutron spectrum is determined in L_2 approximation for a wide range of absorption and the value of E_c is calculated in terms of absorption.

In Part II of our investigations to be published at a later date, the spectrum of thermal neutrons in the cell of a heterogeneous reactor will be considered.

CALCULATION OF NEUTRON THERMALIZATION BY LAGUERRE POLYNOMIALS APPROXIMATION

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Introduction

One of the most important problems in the theory of thermal reactors is the slowing-down and thermalization of neutrons i.e. the neutron energy spectrum in homogeneous and heterogeneous reactors. The slowing down process can be divided into two parts:

1. Slowing-down from fission energy to 1 eV;
2. The setting in of thermal equilibrum, below 1,eV.

During the later process the neutrons get into a state of thermodynamical equilibrium with the atoms of the moderator. The slowing-down and the resulting thermal neutron spectrum form the subject of the theory of neutron thermalization.

These two slowing down regions are rather different as regards both theoretical considerations and experimental investigations. In the first case the effects of the thermal motion of atoms and of chemical bonds are neglected since any collision results in a diminution of neutron energy. In the second case the thermal motion and chemical bonds are taken into account, and the neutrons may either gain or lose energy as a result of scattering.

Strictly speaking there is a third region too between slowing-down and thermalization. This is the transition region which causes the most difficulties from the theoretical viewpoint. In the course of our calculation we disregard this region and assume the thermal region to follow immediately that of slowing-down.

Consequently the qualitative description of the neutron spectra in the two regions can be given as follows:

1. The neutron flux in the slowing-down region above 1eV has the form 1/E.
2. The thermal neutron spectrum is similar to a Maxwellian distribution and may be called quasi-Maxwellian.

In Fig.1. the shape of the spectrum in each region is shown.

The thermal neutron spectrum is considered now in the Laguerre polynomials approximation i.e. we expand the thermal neutron flux into a series of the first kind Laguerre polynomials. Thus an infinite set of equations

is obtained which can be solved approximately by considering only the first n terms. This treatment is called L_{n-1} approximation. We shall use L_1 and L_2 approximations only.

The spectra obtained by this method can be used for calculating the mean values of the absorption cross sections. If the neutron spectra are not known, the artificial notion of the "neutron temperature" is used in the averaging. This "neutron temperature" is generally obtained from an empirical formula of the form

$$T_n = T_{mod}\left[1 + C\frac{\Sigma_a(T_M)}{\xi\,\Sigma_s}\right]$$

where c = 1,1 .... 1,82. The Maxwellian for T_n is used for averaging the absorption cross sections.

If the spectrum is known, there is no need for the "neutron temperature", which is a roughly approximate quantity, for the true thermal neutron spectrum rather differs from a Maxwellian. This is why the calculation of the thermal neutron spectrum is so important.

Of course, the thermal neutron spectrum in a homogeneous infinite medium can be calculated also by other methods than the Laguerre approximation [1] , [2]. However, the latter has some advantages over the others. It is simpler, necessitates less numerical work, and can easily be applied to heterogeneous systems too.

2. The relation between the slowing-down and the quasi-Maxwellian sections of the neutron flux

The basic equation of the theory of neutron spectra is the energy dependent Boltzmann equation:

$$\Omega\nabla\phi(E,\Omega,r) + \Sigma_a(E)\phi(E,\Omega,r) =$$

$$= \int_0^\infty dE' \int_{4\pi} \Sigma_s(E,E',\Omega,\Omega')\,\phi(E',\Omega',r)\,d\Omega' - \Sigma_s(E)\phi(E,\Omega,r) + Q(E,r,\Omega) \qquad /2.1/$$

where Q/E/ is the source of the fission neutrons.

The simplest problem is the neutron spectrum calculation in an infinite homogeneous system. In this case $\phi(E,r,\Omega)$ is independent of the spatial and angular variables, therefore the Eq. /2.1/ can be integrated with respect to r and Ω :

$$[\Sigma_a(E)+\Sigma_s(E)]\Phi(E)=\int_0^\infty \Sigma_s(E'\to E)\Phi(E')\,dE'+Q(E) \qquad /2.2/$$

This equation holds also in the case of a critical reactor. It seems somewhat perplexing that the equation for a reactor contains a source term, although a critical reactor is a source-free system. Considering, however, that the fission neutron spectrum is considerably independent of the spectrum of neutrons inducing fission, the neutrons produced by fission can be considered as a source term. Since the fission energy is well above the thermal energy, we have to consider only the asymptotic solution of /2.2/ i.e. the solution of

$$[\Sigma_a(E)+\Sigma_s(E)]\Phi(E)=\int_0^\infty \Sigma_s(E'\to E)\Phi(E')\,dE' \qquad /2.3/$$

This equation was investigated by several authors for various moderators [1], [2],[3],[4] .

We shall try to solve /2.3/ for the thermal energy range using Laguerre expansion:

$$\Phi(E)=M\left(\frac{E}{T}\right)\sum_{n=0}^{\infty} c_n L_n^{(1)}\left(\frac{E}{T}\right) \qquad /2.4/$$

where $M\left(\frac{E}{T}\right)=\frac{E}{T^2}e^{-\frac{E}{T}}$ is the Maxwellian spectrum at temperature T of the moderator and

$$c_n=\frac{1}{1+n}\int_0^\infty \Phi(E)\,L_n^{(1)}\left(\frac{E}{T}\right)dE \qquad /2.5/$$

$L_n^{(1)}\left(\frac{E}{T}\right)$ is the n-th first kind Laguerre-polynomial. The Laguerre polynomials give an orthogonal system when normalized to

$$\int_0^\infty M\left(\frac{E}{T}\right)L_n^{(1)}\left(\frac{E}{T}\right)L_m^{(1)}\left(\frac{E}{T}\right)dE=(n+1)\delta_{nm} \qquad /2.6/$$

The first three Laguerre polynomials are

$$L_0^{(1)}\left(\frac{E}{T}\right)=1 \;;\quad L_1^{(1)}\left(\frac{E}{T}\right)=2-\frac{E}{T} \;;\quad L_2^{(1)}\left(\frac{E}{T}\right)=3-3\frac{E}{T}+\frac{1}{2}\left(\frac{E}{T}\right)^2$$

One can see from /2.5/ that if for large values of E $\phi \sim 1/E$, then the expansion /2.4/ is meaningless since the integral /2.5/ does not converge even for n = 0. Nevertheless, the method of Laguerre polynomials can be used, all the same, in the following way. Let us divide $\phi(E)$ into two parts:

$$\phi(E)=\phi_T(E)+\phi_L(E) \qquad /2.7/$$

and impose the following conditions

$$\phi_L(E)\sim\frac{1}{E} \qquad E>>T \qquad /2.8a/$$

$$\phi_T(E)=0 \qquad E=0 \qquad /2,8b/$$

$$\phi_T(E)\gg\phi_L(E) \qquad E\sim T \qquad /2.8c/$$

$$\phi_L(E)\gg\phi_T(E) \qquad E>>T \qquad /2.8d/$$

with the assumption that the series /2.1/ of $\phi_T(E)$ converges.

Let us substitute /2.7/ into /2.3/:

$$\left[\Sigma_a(E)+\Sigma_s(E)\right]\phi_T(E)=\int_0^\infty \Sigma_s(E'\to E)\phi_T(E')\,dE'+S(E) \qquad /2.9/$$

Introducing the notation:

$$S(E)=\int_0^\infty \Sigma_s(E'\to E)\phi_L(E')\,dE'-\left[\Sigma_a(E)+\Sigma_s(E)\right]\phi_L(E) \qquad /2.10/$$

S/E/ will be called the slowing-down source.

Let us calculate the slowing-down source, using the assumptions /2.8/ and neglecting some terms.

Let E_c be the energy above which the thermal motion and chemical bonds of the moderator can be neglected, i.e. for $E' > E_c$, $\sum_s(E' \to E)$ is replaced by

$$\sum_s(E' \to E) = \begin{cases} = \dfrac{\sum_{s0}}{\alpha E'} , & (1-\alpha)E' < E < E' \\ = 0 & \text{in every other case} \end{cases} \qquad /2.11/$$

Here $\alpha = \frac{4M}{(M+1)^2}$ and M is the mass of the nucleus. The conditions /2.8c/ and /2.8d/ are satisfied by choosing

$$\Phi_T(E) = 0 \quad \text{if} \quad E > E_c$$
$$\Phi_L(E) = 0 \quad \text{if} \quad E < E_c \qquad /2.12/$$

By /2.12/ the form of the slowing-down source is

$$S(E) = \begin{cases} = \int_0^\infty \sum_s(E' \to E)\, \Phi_L(E')\, dE', & E < E_c \\ = 0 , & \text{if} \quad E > E_c \end{cases} \qquad /2.13/$$

For simplicity the absorption is neglected above E_c./The case without this approximation is considered in App.1./ Thus for $E \geq E_c$

$$\Phi_L(E) = \frac{K_0}{\xi \sum_{s0} E} \quad \text{if} \quad E \geq E_c \qquad /2.14/$$

where $\xi = 1 + \frac{1-\alpha}{\alpha} \log(1-\alpha)$

Substituting /2.11/ and/ 2.14/ into/ 2.13/ :

$$S(E)=\begin{cases} =\int_{E_c}^{\frac{E}{1-\alpha}} \frac{K_0}{\xi\alpha E'^2}\,dE' = \frac{K_0}{\xi\alpha}\left[\frac{1}{E_c}-\frac{1-\alpha}{E}\right], & \text{if} \quad (1-\alpha)E_c \leq E \leq E_c \\ =0 & \text{in every other case} \end{cases} \qquad /2.15/$$

Thus Eq. / 2.9 / has the following form:

$$\left[\Sigma_a(E)+\Sigma_s(E)\right]\Phi_T(E) = \int_0^\infty \Sigma_s(E'\to E)\,\Phi_T(E')\,dE' + \qquad /2.16/$$

$$+\frac{K_0}{\xi\alpha}\left[\frac{1}{E_c}-\frac{1-\alpha}{E}\right]\cdot\varepsilon(E_c,E)$$

where

$$\varepsilon(E_c,E)=\begin{cases} =1 & \text{if} \quad (1-\alpha)E_c \leq E \leq E_c \\ =0 & \text{in every other case} \end{cases}$$

The /2.16/ equation can already be treated by Laguerre polynomials.
Since the $\Phi(E)$ spectrum must be continuous:

$$\Phi_T(E_c) = \Phi_L(E_c) \qquad /2.17/$$

This equation is used for the determination of E_c.

3. The L_1 and L_2 approximation

Let us expand $\Phi(E)$ and S/E/ in series of Laguerre polynomials:

$$\Phi_T(E) = M(E)\sum_{n=0}^{\infty} c_n L_n^{(1)}(E) \qquad /3.1/$$

$$S(E) = M(E)\sum_{n=0}^{\infty} s_n L_n^{(1)}(E)$$

where

$$c_n = \frac{1}{1+n}\int_0^\infty \phi_T(E)\,L_n^{(1)}(E)\,dE$$

$$s_n = \frac{1}{1+n}\int_0^\infty S(E)\,L_n^{(1)}(E)\,dE \qquad /3.2/$$

Substituting /3.1/ into /2.11/ ,multiplying it by $L_m^{(1)}(E)$ and integrating over E, we get:

$$\sum_n c_n \beta_{mn} = \sum_n \gamma_{mn} c_n + s_n \qquad /3.3/$$

We introduce the notations:

$$\beta_{mn} = \int_0^\infty M\left(\frac{E}{T}\right) L_n^{(1)}\left(\frac{E}{T}\right) L_m^{(1)}\left(\frac{E}{T}\right) \Sigma_a(E)\,dE \qquad /3.4a/$$

$$\gamma_{mn} = -\frac{1}{2}\int_0^\infty\int_0^\infty dE\,dE'\,M\left(\frac{E}{T}\right)\Sigma_s(E\to E')\left[L_n^{(1)}(E') - L_n^{(1)}(E)\right]\left[L_m^{(1)}(E') - L_m^{(1)}(E)\right] \qquad /3.4b/$$

For the transformation of γ_{mn} ,we have used the condition of detailed balance:

$$M(E')\Sigma_s(E'\to E) = M(E)\Sigma_s(E\to E')$$

and we see from /3.4b/ that $\gamma_{i0} = 0$.

The set of Eqs. /3.3/ is infinite. We solve it approximately by considering only the first n terms. This is called L_{n+1} approximation. We shall deal with the L_1 and L_2 approximations. E.g. the L_1 equations are the following:

$$c_0\beta_{00} + c_1\beta_{01} = s_0$$

$$c_0\beta_{01} + (\beta_{11} - \gamma_{11})c_1 = s_1 \qquad /3.5/$$

and from /2.10/ and /3.2/ we have

$$s_0 = K_0$$

$$s_1 = K_0\left(1-\frac{1}{4}\,\frac{\alpha}{\xi}\,\frac{E_c}{T}\right) \qquad /3.6/$$

For the case of hydrogeneous moderator

$$s_1 = K_0\left(1-\frac{E_c}{4T}\right) \qquad /3.6'/$$

and for heavy moderators , $\alpha << 1$, $\xi \sim \frac{\alpha}{2}$

$$s_1 = K_0\left(1-\frac{E_c}{2T}\right) \qquad /3.6''/$$

In the following we deal only with the case $\alpha = 1$.

The L_1 equations have an interesting physical meaning. One can show that actually they express the conservation law of the number and energy of neutrons./ See: App.1./

The equations of the L_2 approximation are

$$\beta_{00} C_0 + \beta_{01} C_1 + \beta_{02} C_2 = s_0 \qquad /3.7a/$$

$$\beta_{10} C_0 + (\beta_{11} - \gamma_{11}) C_1 + (\beta_{12} - \gamma_{12}) C_2 = s_1 \qquad /3.7b/$$

$$\beta_{20} C_0 + (\beta_{21} - \gamma_{21}) C_1 + (\beta_{22} - \gamma_{22}) C_2 = s_2 \qquad /3.7c/$$

from /2.15/ and /3.2/

$$s_2 = K_0\left[1-\frac{\alpha}{2\xi}\cdot\frac{E_c}{T} + \frac{\alpha}{12\xi}\left(\frac{E_c}{T}\right)^2\left(1-\frac{\alpha}{3}\right)\right] \qquad /3.6c/$$

In the case of hydrogen: ($\alpha = 1$)

$$s_2 = K_0\left[1-\frac{E_c}{2T} + \frac{1}{18}\left(\frac{E_c}{T}\right)^2\right] \qquad /3.6c'/$$

and for heavy moderators

$$S_2 = K_0\left[1 - \frac{E_c}{T} + \frac{1}{6}\left(\frac{E_c}{T}\right)^2\right] \qquad /3.6c''/$$

4. Results and discussions

We apply the Laguerre polynomials approximation to a moderator of Wigner-Wilkins kernel. That is we assume that

$$\Sigma_s(E' \to E) = \begin{cases} = \frac{\Sigma_{s0}}{E'} \cdot \frac{2}{\sqrt{\pi}} \int_0^{\sqrt{\frac{E}{T}}} e^{-x^2} dx, & \text{if} \quad E' > E \\ = \frac{\Sigma_{s0}}{E'} e^{\frac{E'-E}{T}} \cdot \frac{2}{\sqrt{\pi}} \int_0^{\sqrt{\frac{E'}{T}}} e^{-x^2} dx, & \text{if } E' < E \end{cases} \qquad /4.1/$$

This is the thermal scattering kernel of a monatomic hydrogeneous moderator. It is known that water is similar to a monoatomic hydrogeneous moderator as regards neutron thermalization. It can be explained by the fact that the increasing scattering cross section is compensated by the decreasing energy transfer .[5] .

With the help of /4.1/ one can compute:

$$\gamma_{11} = -1{,}41\,\Sigma_{s0}\,; \quad \gamma_{12} = 0{,}25\,\gamma_{11}\,; \quad \gamma_{22} = 1{,}94\,\gamma_{11}$$

Thus the Eqs. /3.7/ with the condition /2.17/ ,assuming 1/v absorption law„become

$$C_0 + 0{,}5\,C_1 + 0{,}375\,C_2 = 1 \qquad /4.2a/$$

$$0{,}5C_0 + (1{,}75 + \Delta^{-1})C_1 + (0{,}9375 + 0{,}25\Delta^{-1})C_2 = 1 - \frac{E_c}{4T} \qquad /4.2b/$$

$$0{,}375C_0 + (0{,}9375 + 0{,}25\Delta^{-1})C_1 + (2{,}39 + 1{,}94\Delta^{-1})C_2 = 1 - \frac{E_c}{2T} + \frac{1}{18}\left(\frac{E_c}{T}\right)^2 \qquad /4.2c/$$

$$C_0 + 2C_1 + 3C_2 - (C_1 + 3C_2)\frac{E_c}{T} + \frac{1}{2}C_2\left(\frac{E_c}{T}\right)^2 = 1{,}41\Delta\left(\frac{T}{E_c}\right)^2 e^{\frac{E_c}{T}} \qquad /4.2d/$$

where the symbol $\Delta = -\frac{\Sigma_a}{\gamma_{11}}$ and the normalization $\frac{K_0}{\Sigma_a} = 1$ have been used.

Fig.2. shows the E_c cut-off as a function of Δ. In the case of zero absorption, E_c is infinite. This is understandable since there is only a simple Maxwellian in that case, and no 1/E region at all. To have a stationary solution with the absorption tending to zero, the source must also tend to zero.

In Fig.3. the energy yielding the maximum value of $\phi_T(E)$ is shown as a function of Δ .Up to quite large values of Δ the curve is seen to increase monotonously, but eventually this increase ceases and the curve bends back at an extremely large Δ .This bending back is found not only by the Laguerre polynomials approximation, but by numerical integration of the Wigner-Wilkins equation too.

In Fig.4. the $\phi(E)$ can be seen for some values of Δ neutron flux.

In Fig.5. we compare an L_2 spectrum with the empirical [6] ,as well as with the spectrum calculated by numerical integration of the Wigner-Wilkins equation [7] .One can see that the L_2 spectrum is somewhat softer, than that fitted to the experimental points. This is in agreement with the well-known fact that the Wigner-Wilkins equation gives less hardened spectra than required [8] .

We can see all the same that the L_2 approximation gives the spectra relatively well up to $\Sigma_a \cong 0{,}2\ \mathrm{cm}^{-1}$. For greater Σ_a the spectra will be softer than required. In Table 1. the 1/v cross sections are presented as averaged over the spectrum.

For possible improvement let us summarize the approximations involved in our results.

1/ The thermal motion of the moderator atoms above E_c is neglected.

2/ The absorption above E_c is neglected.

3/ Only the first three terms in the Laguerre expansion are considered.

For hydrogen the 1/v absorption above E_c can easily be taken into account. To do this /see App.2/ we only have to use the equation

$$c_0 + 2c_1 + 3c_2 - (c_1 + 3c_2)\frac{E_c}{T} + \frac{1}{2}c_2\left(\frac{E_c}{T}\right)^2 = \frac{1{,}41\,\Delta}{1+\frac{\Sigma_a(E_c)}{\Sigma_{s0}}} \cdot \frac{T^2}{E_c^2}\, e^{\frac{E_c}{T}} \qquad /4.2d'/$$

instead of /4.2d/ .Even for other, heavier moderators the 1/v absorption can be taken into account but the result will be more complicated. From /4.2d'/ one can see that the correction term would be significant only in the case of rather strong absorption.

In order to get rid of the consequences of the first approximation we have to consider the transition region. E.g. an approximate way would be the expansion of $\Sigma_s(E' \to E)$ and $\phi_L(E)$ into a power series in 1/E /see [9] .

The error due to the truncation of the Laguerre series can be diminished by using the L_3, L_4..... etc. approximations.Use of higher order approximations, however, is too laborious, and in this case simplicity, the

main advantage of the Laguerre-approximation would be lost. The other reason for not using higher order approximations are errors involved in approximations 1/, 2/, which may be larger than that due to the truncation in L_2 approximation.

A further advantage of the Laguerre approximation is that the kernel $\sum_s(E' \to E)$ has not to be fully known. The knowledge of γ's is sufficient, e.g. the L_1 approximation necessitates only the knowledge of γ_{11} which can be obtained experimentally from the so-called diffusion cooling [10]

Table 1.

$\sigma_a \left[\frac{\text{barn}}{\text{H-atom}}\right]$	0,332	3,15	6,04
$\sum_a [\text{cm}^{-1}]$	0,0195	0,1893	0,3629
$\frac{\bar{\sigma}_{a\,\text{calc}}^{L_2\text{-appr}}}{\bar{\sigma}_{a\,\text{meas}}}$	1,004	1,062	1,089
$\frac{\bar{\sigma}_{a\,\text{calc.}}^{\text{Maxwell}}}{\bar{\sigma}_{a\,\text{meas}}}$	1,005	1,112	1,13

where

$$\bar{\sigma}_{a\,\text{calc}}^{\text{Maxwell}} = \sigma_a(2200)\frac{\sqrt{\pi}}{2}\sqrt{\frac{293,6}{T_n}}$$

and

$$T_n = T_{\text{Mod}}\left[1+1,815\,\frac{\sum_a(T_M)}{\sum_s}\right]$$

Appendix 1.

The physical meaning of the L_1 approximation

Eq./ 3.5a/ can be obtained by integrating/ 2.9/ over E

$$\int_0^\infty \Sigma_a(E)\Phi_T(E)dE = \int_0^\infty s(E)dE \qquad /1/$$

Thus the first L_1 equation expresses the fact of neutron number conservation.

Multiplying now Eq. / 3.5a/ by two, and subtracting Eq. / 3.5b/ , we get:

$$\int_0^\infty E\Sigma_a(E)\Phi_T(E)dE = \int_0^\infty (E-E')\Sigma_s(E'\to E)\Phi_T(E')dE'dE + \int_0^\infty Es(E)dE \qquad /2/$$

This expresses the law of energy conservation. Starting from these two laws of conservation, and making use of the relation

$$\frac{E_c}{T_{eff}^2}\, e^{-\frac{E_c}{T_{eff}}} = \frac{konst}{E_c} \qquad /3/$$

instead of /2.17/ Galanin [11] has determined the so-called T_{eff} "neutron temperature".

Let us introduce the notation $x = \frac{T_{eff}-T}{T_{eff}} \approx \frac{T_{eff}-T}{T}$ and expand the exponential term in Eq. / 3/ up to the linear term

$$\left(\frac{1}{T_{eff}^2} \approx \frac{1}{T^2}(1-2x)\right)$$

$$\frac{E_c}{T^2}\, e^{-\frac{E_c}{T}}\left(1-2x+\frac{E_c}{T}x\right) = \frac{konst}{E_c} \qquad /3'/$$

If we define the neutron temperature as

$$T_{eff} = \frac{1}{2}\,\frac{\int_0^\infty \Phi_T(E)E\,dE}{\int_0^\infty \Phi_T(E)\,dE} = T\left(1-\frac{C_1}{C_0}\right) \qquad /4/$$

then, writing this into Eq. / 3'/ , we shall get an equation identical to /2.17/ .

Appendix 2.

1/v absorption above E_c in the case of hydrogen

It is known that for hydrogen

$$\Phi_L(E) = \frac{K_0}{\Sigma_a + \Sigma_s} e^{-\int_0^\infty \frac{\Sigma_a}{\Sigma_a + \Sigma_s} \cdot \frac{dE}{E'}}$$

Performing the integration we get

$$\Phi_L(E) = \frac{K_0}{\Sigma_s \left(1 + \frac{\Sigma_a}{\Sigma_s}\right)^3 E}$$

Thus

$$S(E) = \int_0^\infty \frac{K_0 dE}{\Sigma_s \left(1 + \frac{\Sigma_a}{\Sigma_s}\right)^3 E^2} = \frac{K_0}{E_c} \cdot \frac{1}{\left(1 + \frac{\Sigma_a(E_c)}{\Sigma_s}\right)^3}$$

From this we can obtain the values of s_0, s_1, s_2. They will differ from /3.6'/ in that K_0 is always replaced by $\frac{K_0}{\left(1 + \frac{\Sigma_a(E_c)}{\Sigma_s}\right)^2}$ If we normalize with $\frac{K_0}{\left(1 + \frac{\Sigma_a(E_c)}{\Sigma_s}\right)^2}$ instead of K_0, then we have again /4.2/

Appendix 3.

Formulae /3.6/ for mixtures

The formulae /3.6/ can easily be generalized for mixtures. The formula /2.11/ for mixtures is given by

$$\sum_s (E' \to E) = \sum_i \frac{\Sigma_{soi}}{\alpha_i E'} \varepsilon(\alpha_i E E') = \sum_i \Sigma_{si}(E' \to E)$$

where

$$\hat{\varepsilon}(\alpha_i) = \begin{cases} = 1, & \text{if} \quad (1-\alpha_i) E' < E < E' \ ; \\ = 0 & \text{in every other case} \end{cases}$$

Thus /2,13/ will become

$$S(E) = \begin{cases} = \sum_i \int_0^\infty \Sigma_{si}(E' \to E) \phi_L(E')\, dE' & \text{if} \quad E < E_c \\ = 0 & \text{in every other case} \end{cases}$$

and from Eq. /2.14/ we have

$$\phi_L(E) = \frac{K_0}{\bar{\xi} \bar{\bar{\Sigma}}_{so} E} \qquad \text{if} \qquad E > E_c$$

where

$$\bar{\xi} = \frac{\sum_i \xi_i \Sigma_{soi}}{\sum_i \Sigma_{soi}} \ ; \quad \bar{\bar{\Sigma}}_{so} = \sum_i \Sigma_{soi}$$

Thus by /2.15/

$$S(E) = \frac{K_0}{\bar{\xi} \bar{\bar{\Sigma}}_{so}} \sum_i \frac{\Sigma_{soi}}{\alpha_i} \left(\frac{1}{E_c} - \frac{1-\alpha_i}{E} \right) \varepsilon(\alpha_i, E, E_c)$$

Consequently the formula /3,6/ can be written as

$$s_0 = K_0 \ ; \quad s_1 = K_0 \left(1 - \frac{1}{4} \frac{\bar{\alpha}}{\bar{\xi}} \cdot \frac{E_c}{T} \right) \ ;$$

$$s_2 = K_0 \left[1 - \frac{1}{2} \frac{\bar{\alpha}}{\bar{\xi}} \frac{E_c}{T} + \frac{1}{12 \bar{\xi}} \left(\bar{\alpha} - \frac{\bar{\alpha}^2}{3} \right) \left(\frac{E_c}{T} \right)^2 \right]$$

where

$$\bar{\alpha} = \frac{\sum_i \Sigma_{soi} \alpha_i}{\bar{\bar{\Sigma}}_{so}} \ ; \qquad \bar{\alpha}^2 = \frac{\sum_i \Sigma_{soi} \alpha_i^2}{\bar{\bar{\Sigma}}_{so}}$$

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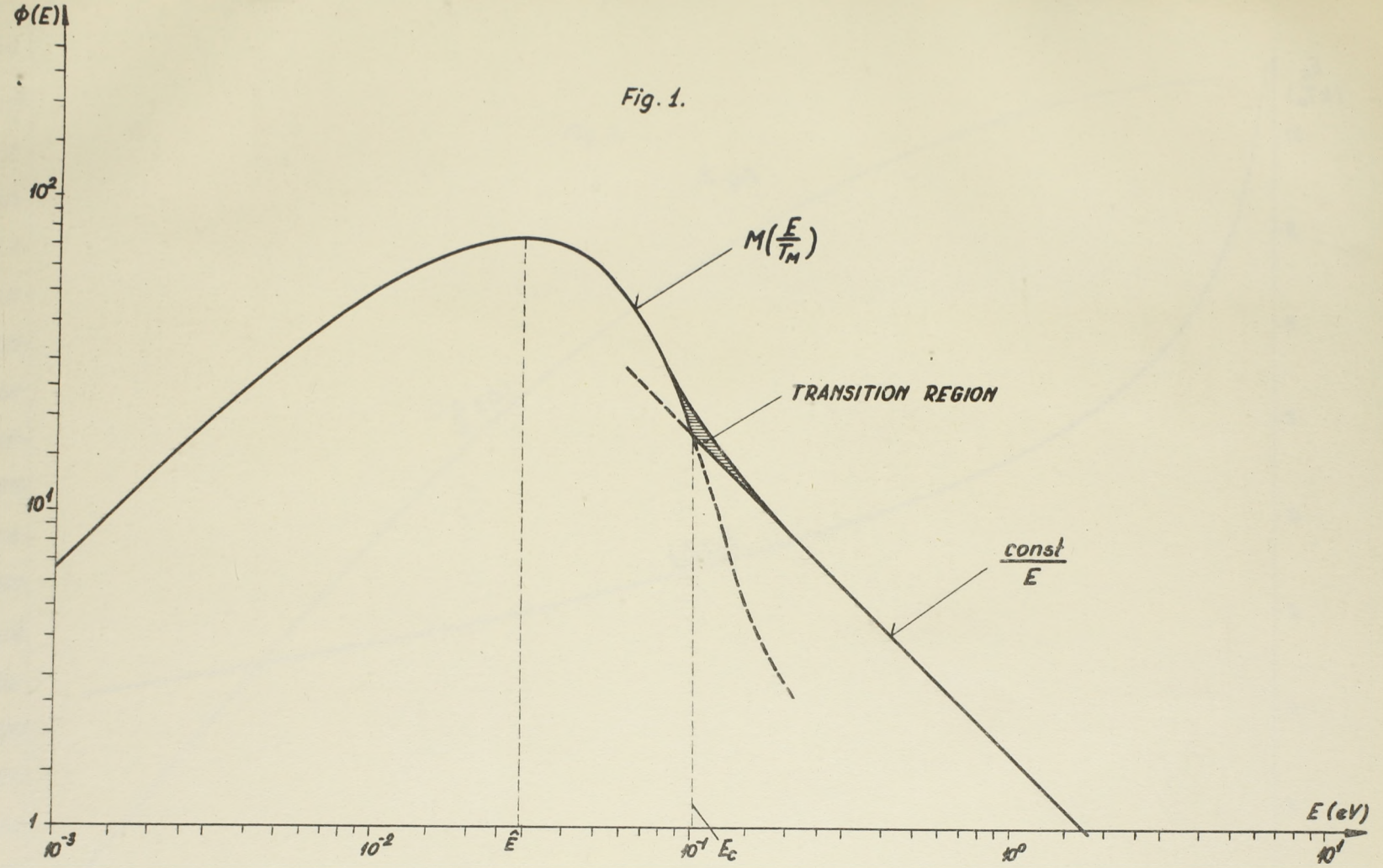
Fig. 1.


$\phi(E)$
10^2
10^1
1
$M(\frac{E}{T_M})$
TRANSITION REGION
$\frac{const}{E}$
10^{-3}
10^{-2}
$\hat{E}$
10^{-1}
E_c
10^0
10^1
E (eV)

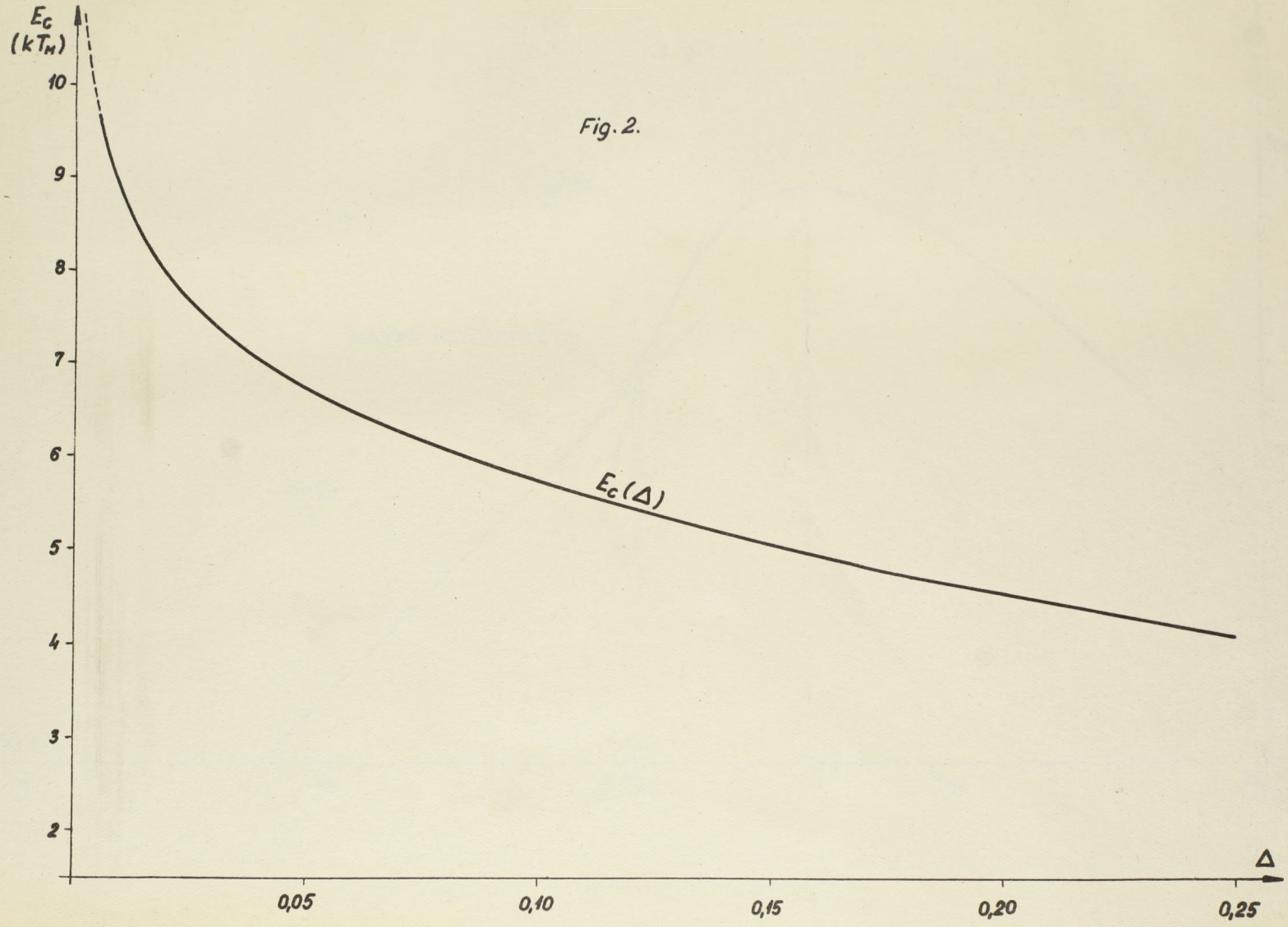


Fig. 2.

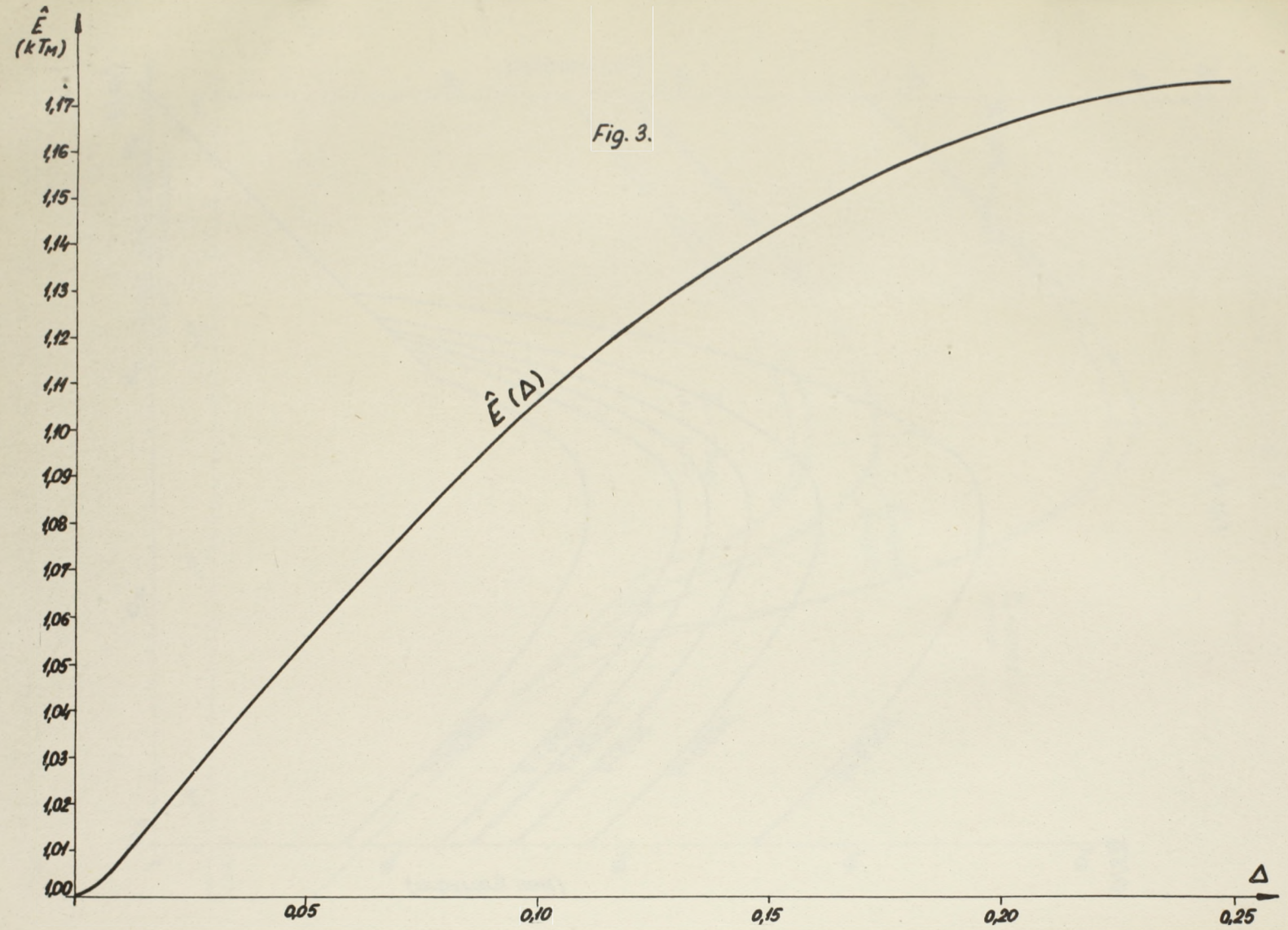

$\hat{E}$ / (kT_M)
1,17
1,16
1,15
1,14
1,13
1,12
1,11
1,10
1,09
1,08
1,07
1,06
1,05
1,04
1,03
1,02
1,01
1,00
$\hat{E}(\Delta)$
0,05
0,10
0,15
0,20
0,25
Δ

Fig. 3.

Fig. 4.

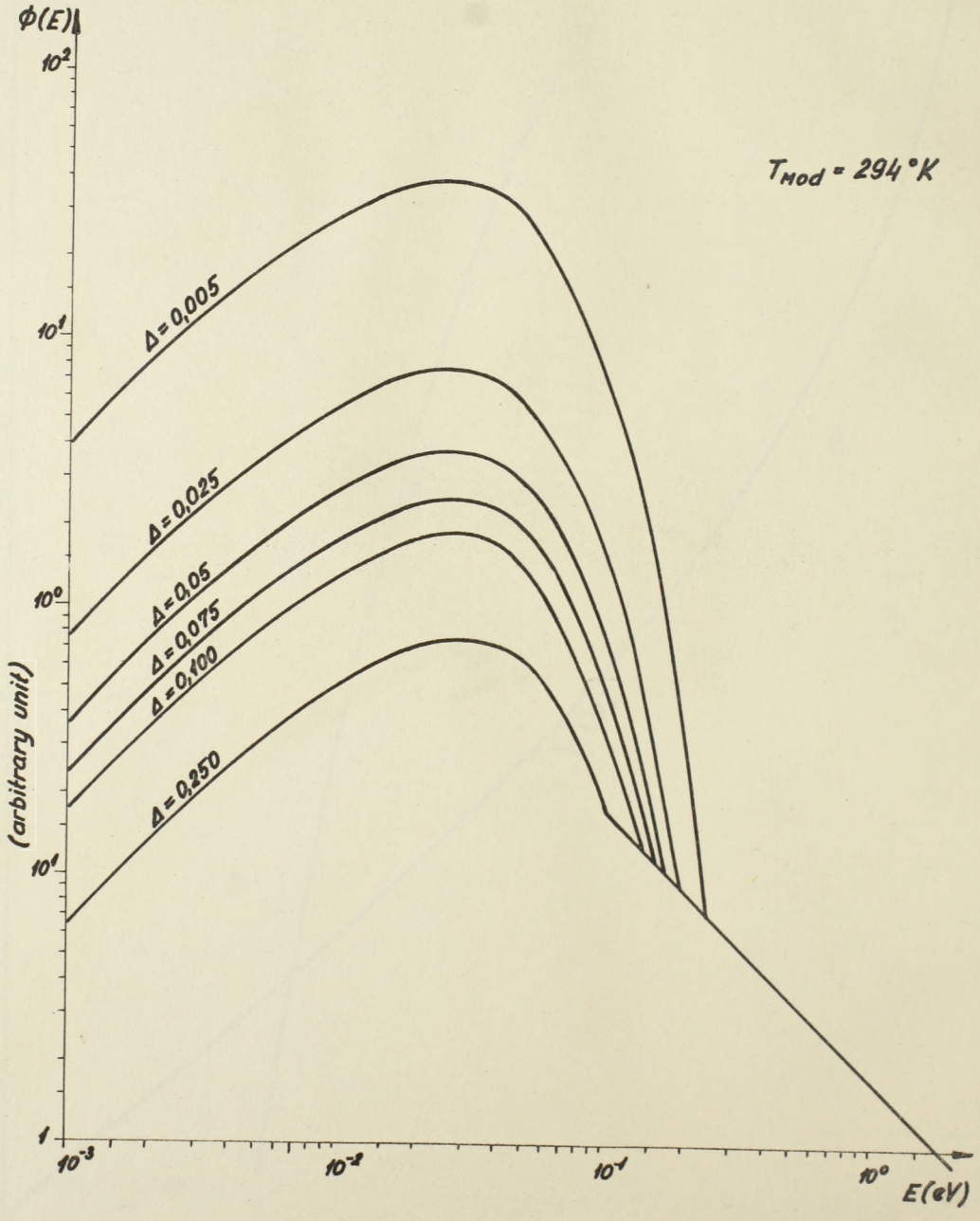
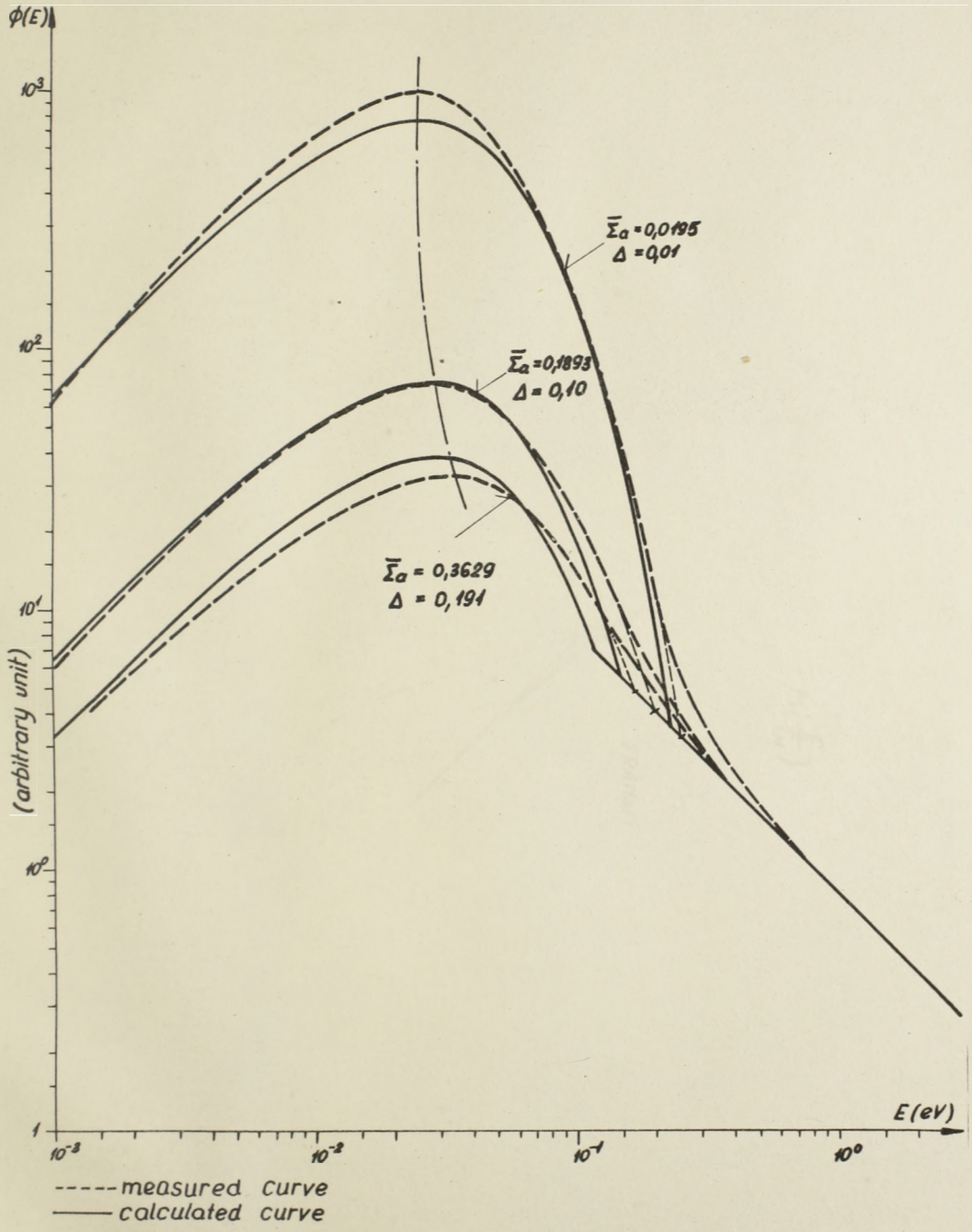

Φ(E)
10²
10¹
10⁰
10⁻¹
1
(arbitrary unit)
T_Mod = 294 °K
Δ = 0,005
Δ = 0,025
Δ = 0,05
Δ = 0,075
Δ = 0,100
Δ = 0,250
10⁻³
10⁻²
10⁻¹
10⁰
E(eV)

Fig. 5.


φ(E)
10³
10²
10¹
10⁰
1
(arbitrary unit)
Σ̄a = 0,0195
Δ = 0,01
Σ̄a = 0,1893
Δ = 0,10
Σ̄a = 0,3629
Δ = 0,191
10⁻³
10⁻²
10⁻¹
10⁰
E (eV)
----- measured curve
—— calculated curve